The sum of the squares of degrees: an overdue assignement

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Abstract

Let $f(n,m)$ be the maximum of the sum of the squares of degrees of a graph with n vertices and m edges. Summarizing earlier research, we present a concise, asymptotically sharp upper bound on $f(n,m)$, better than the bound of de Caen for almost all n and m.

Keywords: *squares of degrees, de Caen's bound, sharp bound*

1 Introduction

Our notation is standard (e.g., see [3]). Specifically, in this note, n and m denote the number of vertices and edges of a graph G.

Few problems in combinatorics have got so many independent solutions as the problem of finding

$$f(n,m)=\max\left\{\sum_{u\in V(G)}d^2(u):v(G)=n,\ e(G)=m\right\}.$$

The first contribution is due to B. Schwarz [11] who studied how to shuffle the entries of a square nonnegative matrix A in order to maximize the sum of the entries of A^2. Later M. Katz [9] almost completely solved the same problem for square $(0,1)$-matrices, obtaining, in particular, an asymptotic value of $f(n,m)$. The first exact result for $f(n,m)$, found in 1978 by Ahlswede and Katona [2], reads as: suppose r,q,s,t are integers defined uniquely by

$$m=\binom{r}{2}+q=\binom{n}{2}-\binom{s}{2}-t,\quad 0\leq q<r,\ 0\leq t<s, \tag{1}$$

and set

$$C(n,m)=2m(r-1)+q(q+1), \tag{2}$$

$$S(n,m)=(n(n-1)-2m)(s-1)+t(t+1)+4m(n-1)-(n-1)^2n. \tag{3}$$

Then

$$f(n,m) = \max\{C(n,m), S(n,m)\}. \tag{4}$$

Moreover, Ahlswede and Katona demonstrated that, if $|m - n(n-1)/4| < n/2$, finding $\max\{C(n,m), S(n,m)\}$ is a subtle and difficult problem; hence, there is little hope for a simple exact expression for $f(n,m)$.

Almost at the same time Aharoni [1] completed the work of Katz for square $(0,1)$-matrices. In 1987 Brualdi and Solheid [5], adapting Aharoni's method to graphs, rediscovered (4) and in 1996 Olpp [10], apparently unaware of these achievements, meticulously deduced (4) from scratch.

Despite this impressive work, none of these authors came up with a concise, albeit approximate upper bound on $f(n,m)$. In contrast, de Caen [6] proved that

$$f(n,m) \leq m\left(\frac{2m}{n-1} + n - 2\right). \tag{5}$$

Denote the right-hand side of (5) by $D(n,m)$ and note that, for almost all n and m, it is considerably greater than $f(n,m)$ - in fact, for m around $n^2/4$ and n sufficiently large, $D(n,m) > 1.06 f(n,m)$. De Caen was aware that $D(n,m)$ matches $f(n,m)$ poorly, but he considered that it has "... an appealingly simple form." He was right - his result motivated further research, e.g., see [4], [7], and [8]. Sadly enough, neither de Caen, nor his successors refer to the work done before Olpp.

In summary: the result (4) is exact but complicated, while de Caen's result (5) is simple but inexact.

The aim of this note is to find a concise, asymptotically sharp upper bound on $f(n,m)$, better than de Caen's bound for almost all n and m.

We begin with the following "half" result.

Theorem 1 *If $m \geq n(n-1)/4$, then*

$$m\sqrt{8m+1} - 3m \leq f(n,m) \leq m\sqrt{8m+1} - m. \tag{6}$$

Moreover, for $m < (n-1)(n-2)/2$,

$$m\sqrt{8m+1} - m < D(n,m). \tag{7}$$

This theorem is almost as good as one can get, but it holds only for half of the range of m. Since

$$f\left(n, \frac{n(n-1)}{2} - m\right) = f(n,m) + 4(n-1)m - n(n-1)^2,$$

one can produce a bound when $m < n(n-1)/4$ as well. We state below a simplified complete version.

Theorem 2 *Let*

$$F(n,m) = \begin{cases} (2m)^{3/2}, & if\ m \geq n^2/4 \\ (n^2 - 2m)^{3/2} + 4mn - n^3, & if\ m < n^2/4. \end{cases}$$

Then, for all n *and* m,

$$F(n,m) - 4m \leq f(n,m) \leq F(n,m). \tag{8}$$

Moreover, if $n^{3/2} < m < \binom{n}{2} - n^{3/2}$, *then*

$$F(n,m) < D(n,m). \tag{9}$$

2 Proofs

To begin with, note that (2) and (3) imply that

$$S(n,m) = C\left(n, \frac{n(n-1)}{2} - m\right) + 4m(n-1) - n(n-1)^2. \tag{10}$$

We need some preliminary results.

Proposition 3 *For all* n *and* $m > 0$,

$$(2m)^{3/2} - 3m < m\sqrt{8m+1} - 3m \leq C(n,m). \tag{11}$$

Proof Let $m = \binom{r}{2} + q$, $0 \leq q < r$. From

$$(8m)^{1/2} < \sqrt{8m+1} = \sqrt{4r(r-1) + 8q + 1} < 2r + 1$$

and (2) we deduce that

$$C(n,m) = 2m(r-1) + q(q+1) \geq 2m\left(r + \frac{1}{2}\right) - 3m \geq m\sqrt{8m+1} - 3m,$$

proving (11) and the proposition. $\square$

Proposition 4 *For every* $r \geq 3$

$$\sqrt{(2r-1)^2 + 8(r-1)} > \frac{2r^2 + 5r - 2}{r+2}.$$

Proof Since
$$\sqrt{(2r-1)^2+8(r-1)}=\sqrt{(2r+1)^2-8},$$
the desired inequality follows from

$$\begin{aligned}(2r+1)^2-8 &\geq (2r+1)^2-8\frac{2r^2+5r}{(r+2)^2}\geq (2r+1)^2-8\frac{(2r+1)(r+2)-2}{(r+2)^2}\\ &=(2r+1)^2-\frac{8(2r+1)}{r+2}+\frac{16}{(r+2)^2}=\left(\frac{2r^2+5r-2}{r+2}\right)^2,\end{aligned}$$

completing the proof. □

Lemma 5 *For all n and m,*

$$C(n,m)\leq m\sqrt{8m+1}-m.$$

Proof Let $m=\binom{r}{2}+q$, $0\leq q<r$. In view of (1) and (2), the required inequality is equivalent to

$$2r(r-1)^2+4rq+2q(q-1)\leq (r(r-1)+2q)\sqrt{(2r-1)^2+8q}-r(r-1)-2q,$$

and so, to

$$(2r-1)r(r-1)\leq (r(r-1)+2q)\sqrt{(2r-1)^2+8q}-4rq-2q^2. \tag{12}$$

It is immediate to check that (12) holds if $r=1$; thus we shall assume that $r\geq 2$. If $q=r-1$, then Proposition 4 implies (12) by

$$\begin{aligned}&(r(r-1)+2(r-1))\sqrt{(2r-1)^2+8(r-1)}-4r(r-1)-2(r-1)^2\\ &=(r-1)\left((r+2)\sqrt{(2r-1)^2+8(r-1)}-6r+2\right)\\ &>(r-1)\left(2r^2+5r-2-6r+2\right)=(r-1)r(2r-1).\end{aligned}$$

Assume now $r\geq 2$, and $0\leq q\leq r-2$. Then Bernoulli's inequality implies that

$$\begin{aligned}\left((2r-1)^2+8q\right)^{3/2} &\geq (2r-1)^3\left(1+\frac{12q}{(2r-1)^2}\right)=(2r-1)^3+12q(2r-1),\\ \left((2r-1)^2+8q\right)^{1/2} &\leq (2r-1)\left(1+\frac{4q}{(2r-1)^2}\right)=(2r-1)+\frac{4q}{(2r-1)},\end{aligned}$$

and so,

$$
\begin{aligned}
&\left(r\left(r-1\right)+2q\right)\sqrt{\left(2r-1\right)^{2}+8q}-4rq-2q^{2}\\
&=\frac{1}{4}\left(\left(2r-1\right)^{2}+8q\right)^{3/2}-\frac{1}{4}\left(\left(2r-1\right)^{2}+8q\right)^{1/2}-4rq-2q^{2}\\
&>\frac{\left(2r-1\right)^{3}+12q\left(2r-1\right)}{4}-\frac{\left(2r-1\right)}{4}-\frac{q}{\left(2r-1\right)}-4rq-2q^{2}\\
&=\left(2r-1\right)r\left(r-1\right)+q\left(2r-3-2q-\frac{1}{\left(2r-1\right)}\right)\\
&\geq\left(2r-1\right)r\left(r-1\right)+q\left(2r-3-2\left(r-2\right)-\frac{1}{\left(2r-1\right)}\right)\geq\left(2r-1\right)r\left(r-1\right).
\end{aligned}
$$

This completes the proof of (12) and of Lemma 5. $\square$

Proof of Theorem 1 The first inequality in (6) follows from $C\left(n,m\right)\leq f\left(n,m\right)$ and Proposition 3. To prove the second inequality in (6), set first

$$A\left(n,m\right)=\left(\frac{n\left(n-1\right)}{2}-m\right)\sqrt{\left(2n-1\right)^{2}-8m}-\frac{n\left(n-1\right)}{2}+m+4m\left(n-1\right)-n\left(n-1\right)^{2}$$

and observe that (10) and Lemma 5 imply that, for all n and m,

$$S\left(n,m\right)\leq A\left(n,m\right). \tag{13}$$

We shall prove that, if $m\geq n\left(n-1\right)/4$, then

$$A\left(n,m\right)\leq m\sqrt{8m+1}. \tag{14}$$

Setting $x=\frac{n(n-1)}{2}-m$, this is equivalent to: if $x\leq n\left(n-1\right)/4$, then

$$
\begin{aligned}
&x\sqrt{8x+1}-x-4x\left(n-1\right)+n\left(n-1\right)^{2}\\
&\leq\left(\frac{n\left(n-1\right)}{2}-x\right)\sqrt{8\left(\frac{n\left(n-1\right)}{2}-x\right)+1}-\frac{n\left(n-1\right)}{2}+x.
\end{aligned}
\tag{15}
$$

Setting $g\left(x\right)=x\sqrt{8x+1}-\left(2n-1\right)x$, (15) is equivalent to: if $0\leq x\leq n\left(n-1\right)/4$, then

$$g\left(x\right)\leq g\left(\frac{n\left(n-1\right)}{2}-x\right)$$

Since,

$$g'\left(x\right)=\sqrt{8x+1}+4x\left(8x+1\right)^{-1/2}-\left(2n-1\right)\geq4x\left(8x+1\right)^{-1/2}>0,$$

$g\left(x\right)$ increases with x, and $g\left(\frac{n(n-1)}{2}-x\right)$ decreases with x. Hence,

$$g\left(x\right)\leq g\left(n\left(n-1\right)/4\right)\leq g\left(\frac{n\left(n-1\right)}{2}-x\right),$$

proving (15) and (14). Finally, if $m \geq n(n-1)/4$, then Lemma 5, 13, and (14) imply that

$$\max\{C(n,m), S(n,m)\} \leq \max\left\{m\sqrt{8m+1}-m, A(n,m)\right\} = m\sqrt{8m+1}-m.$$

This, in view of (4), completes the proof of the second inequality in (6).

Proof of (7)

To prove (7), assume that $m\sqrt{8m+1}-m \geq D(n,m)$. Then

$$\frac{2m}{n-1}+n-1 \leq \sqrt{8m+1}$$

and so,

$$4m^2-4m(n-1)^2+n(n-1)^2(n-2) \leq 0,$$

implying that

$$\frac{2m}{n-1} \geq n-2,$$

a contradiction with the assumption about m. This completes the proof of Theorem 1. □

To simplify the proof of Theorem 2, we need the following lemma.

Lemma 6 *For $m \leq n^2/4$,*

$$S(n,m) \leq \left(n^2-2m\right)^{3/2}+4mn-n^3. \tag{16}$$

Proof Let $\binom{n}{2}-m=\binom{s}{2}+t$. Lemma 5 implies that

$$\begin{aligned} C\left(n,\binom{n}{2}-m\right) &= 2\left(\binom{n}{2}-m\right)(s-1)+t(t+1) \\ &\leq \left(\binom{n}{2}-m\right)\sqrt{(2n-1)^2-8m}-\binom{n}{2}+m. \end{aligned}$$

Hence, in view of (10), inequality (16) follows from

$$\begin{aligned} &\left(\binom{n}{2}-m\right)\sqrt{(2n-1)^2-8m}-\binom{n}{2}+m+4m(n-1)-(n-1)^2 n \\ &\leq \left(n^2-2m\right)^{3/2}+4mn-n^3, \end{aligned}$$

in turn, equivalent to

$$2\left(n^2-2m\right)^{3/2}-(n(n-1)-2m)\sqrt{(2n-1)^2-8m}+6m-3n^2+3n \geq 2n. \tag{17}$$

Thus, our goal is the proof of (17). Note the for $n \leq 3$, inequality (17) holds for every m, so we shall assume that $n \geq 4$. Let

$$g(x)=2(x+n)^{3/2}-x(4x+1)^{1/2}-3x$$

and observe that (17) is equivalent to $g\left(n\left(n-1\right)-2m\right)\geq 2n$. We first prove that $g\left(x\right)$ is decreasing for $n\left(n-1\right)-n^2/2\leq x\leq n\left(n-1\right)$. Indeed,

$$\begin{aligned}
g'\left(x\right) &= 3\left(x+n\right)^{1/2}-\left(4x+1\right)^{1/2}-2x\left(4x+1\right)^{-1/2}-3\\
&= 3\left(x+n\right)^{1/2}-\left(4x+1\right)^{1/2}-2x\left(4x+1\right)^{-1/2}-3\\
&\leq 3x^{1/2}\left(1+\frac{n}{2x}\right)-\frac{6x+1}{\sqrt{4x+1}}-3\leq 3x^{1/2}\left(1+\frac{n}{2x}\right)-\frac{6x+1}{2x^{1/2}\left(1+1/8x\right)}-3\\
&= 3x^{1/2}+\frac{3n}{2x^{1/2}}-\frac{24x+4}{8x+1}x^{1/2}-3<3x^{1/2}+\frac{3n}{2x^{1/2}}-3x^{1/2}-3\\
&= 3\frac{n}{2x^{1/2}}-3=\frac{3}{x^{1/2}}\left(\frac{n}{2}-\left(\frac{n^2}{2}-n\right)^{1/2}\right)<\frac{3}{x^{1/2}}\left(\frac{n}{2}-\frac{n}{\sqrt{2}}\left(1-\frac{1}{n}\right)\right)<0.
\end{aligned}$$

Therefore,

$$g\left(n\left(n-1\right)-2m\right)\geq g\left(n\left(n-1\right)\right)=2n^3-n\left(n-1\right)\left(2n-1\right)-3n\left(n-1\right)=2n,$$

proving (17) and Lemma 6. $\square$

Proof of Theorem 2 Our first goal is to prove the second inequality in (8). Note that the function $g\left(x\right)=x^{3/2}-x$ is increasing for $1/2\leq x\leq 1$. Indeed, $g'\left(x\right)=\frac{3}{2}x^{1/2}-1>\frac{3}{2\sqrt{2}}-1>0$. Hence, $g\left(1-x\right)$ is decreasing for $1/2\leq x\leq 1$. Hence, if $1/2\leq x\leq 1$, then

$$g\left(x\right)\geq g\left(1/2\right)\geq g\left(1-x\right);$$

likewise, if $0\leq x\leq 1/2$, then

$$g\left(1-x\right)\geq g\left(1/2\right)\geq g\left(x\right).$$

Therefore, setting $x=2m/n^2$, we see that, if $n^2/4\leq m\leq n\left(n-1\right)$, then

$$\left(2m\right)^{3/2}\geq\left(n^2-2m\right)^{3/2}+4mn-n^3$$

and, if $0\leq m\leq n^2/4$, then

$$\left(2m\right)^{3/2}\leq\left(n^2-2m\right)^{3/2}+4mn-n^3.$$

In other words,

$$F\left(n,m\right)=\max\left\{\left(2m\right)^{3/2},\left(n^2-2m\right)^{3/2}+4mn-n^3\right\}.$$

Lemma 5 implies that, for all n and m,

$$C\left(n,m\right)\leq m\sqrt{8m+1}-m\leq\left(2m\right)^{3/2};$$

Lemma 6 implies that, for $m\leq n^2/4$,

$$S\left(n,m\right)\leq\left(n^2-2m\right)^{3/2}+4mn-n^3,$$

and so, in view of (4), the second inequality in (8) is proved.

Proof of the first inequality in (8)

To prove the first inequality in (8), assume first that $m < n^2/4$; we shall prove that

$$\left(n^2 - 2m\right)^{3/2} - n^3 + 4mn - 4m \leq S\left(n, m\right).$$

Letting $\binom{n}{2} - m = \binom{s}{2} + t$, in view of (3), this is equivalent to

$$\left(n^2 - 2m\right)^{3/2} \leq \left(n\left(n-1\right) - 2m\right)\left(s-1\right) + t\left(t+1\right) + 2n^2 - n, \tag{18}$$

Thus, our goal is to prove (18).

Bernoulli's inequality implies that

$$\begin{aligned}\left(n\left(n-1\right) - 2m\right)^{3/2} &= \left(n^2 - 2m\right)^{3/2}\left(1 - \frac{n}{n^2 - 2m}\right)^{3/2} \\ &\geq \left(n^2 - 2m\right)^{3/2}\left(1 - \frac{3n}{2\left(n^2 - 2m\right)}\right) = \left(n^2 - 2m\right)^{3/2} - \frac{3}{2}n\left(n^2 - 2m\right)^{1/2},\end{aligned}$$

and so,

$$\left(n^2 - 2m\right)^{3/2} \leq \left(n\left(n-1\right) - 2m\right)^{3/2} + \frac{3}{2}n\sqrt{n^2 - 2m} \leq \left(n\left(n-1\right) - 2m\right)^{3/2} + \frac{3\sqrt{2}}{4}n^2. \tag{19}$$

On the other hand, from

$$n\left(n-1\right) - 2m = s\left(s-1\right) + 2t < s\left(s+1\right)$$

we see that $\sqrt{n\left(n-1\right) - 2m} < s + 1/2$. Hence, in view of (19), we have

$$\begin{aligned}\left(n^2 - 2m\right)^{3/2} &\leq \left(n\left(n-1\right) - 2m\right)\left(s-1\right) + \frac{3}{2}\left(n\left(n-1\right) - 2m\right) + \frac{3\sqrt{2}}{4}n^2 \\ &\leq \left(n\left(n-1\right) - 2m\right)\left(s-1\right) + \frac{3}{2}n\left(n-1\right) - \frac{3n^2}{4} + \frac{3\sqrt{2}}{4}n^2 \\ &< \left(n\left(n-1\right) - 2m\right)\left(s-1\right) + 2n^2 - n,\end{aligned}$$

completing the proof of (18). Since, by Proposition 3, we have

$$\left(2m\right)^{3/2} - 3m \leq C\left(n, m\right),$$

it follows that

$$F\left(n, m\right) - 4m \leq \begin{cases} C\left(n, m\right), & if\ m \geq n^2/4 \\ S\left(n, m\right), & if\ m < n^2/4. \end{cases}$$

implying the first inequality in (8).

Proof of (9)

To prove (9), suppose first that $n^2/4 \le m < \binom{n}{2} - (n-1)^{3/2}$; then we have to prove that

$$(2m)^{3/2} < m\left(\frac{2m}{n-1} + n - 2\right) \tag{20}$$

Assuming that (20) fails, we see that

$$2\sqrt{2m} \ge \frac{2m}{n-1} + n - 2,$$

and so,

$$\left(\sqrt{\frac{2m}{n-1}} - \sqrt{n-1}\right)^2 \le 1.$$

After some algebra we obtain

$$2m \ge n(n-1) - 2(n-1)\sqrt{n-1},$$

a contradiction with the range of m.

Suppose now that $n^{3/2} < m \le n^2/4$. This implies

$$n^2 - 2(n-1)^{3/2} > n^2 - 2m > n^2/2,$$

and thus, by (20),

$$\left(n^2 - 2m\right)^{3/2} < \left(n^2 - 2m\right)\left(\frac{2\left(n^2 - 2m\right)}{n-1} + n - 2\right).$$

Hence,

$$\begin{aligned}
&\left(n^2 - 2m\right)^{3/2} + 4mn - n^3 \\
&< \frac{\left(n^2 - 2m\right)}{2}\left(\frac{\left(n^2 - 2m\right)}{n-1} + n - 2\right) + 4mn - n^3 \\
&= \frac{n^4 - 4mn^2 + 4m^2}{2(n-1)} + \frac{\left(n^2 - 2m\right)}{2}(n-2) + 4mn - n^3 \\
&= -\frac{n^2}{2}\frac{n-2}{n-1} - \frac{2(n-2)m}{(n-1)} + \frac{2m^2}{n-1} + (n-2)m \\
&= \frac{n(n-2)}{(n-1)}\left(2m - \frac{n^2}{2}\right) + \frac{2m^2}{n-1} + (n-2)m < \frac{2m^2}{n-1} + (n-2)m.
\end{aligned}$$

This completes the proof of (9) and of Theorem 2. $\square$

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